Symmetric charge transfer to multiply charged ions

J. N. Bardsley
Lawrence Livermore National Laboratory, Livermore, California 94550

P. Gangopadhyay
Space Science Center, University of Southern California, Los Angeles, California 90089

B. M. Penetrante
Lawrence Livermore National Laboratory, Livermore, California 94550

(Received 27 February 1989)

The asymptotic theory of symmetric charge transfer is adapted to apply to ion-ion collisions through allowance for curved nuclear trajectories. The theory compares well with *ab initio* quantum calculations on He^{2+}-He^{+} collisions and is applied to five members from each of the Li-like and Na-like sequences.

In this paper we will consider the symmetric charge transfer reactions

$$X^{(p-1)+}+X^{p+}\rightarrow X^{p+}+X^{(p-1)+} \ . \tag{1}$$

The motivation for this work arose from studies of the behavior of a plasma injected at high velocity into a stationary plasma in which magnetic fields are present. Coulomb collisions between ions and electrons and the magnetic forces both lead to a coupling between the ions which slows down the injected ions and accelerates the ambient ions. The strength of this coupling is proportional to the ionic charge. Several stages of ionization will usually be produced through ion-ion or ion-electron collisions and one might expect that the different charge states will separate, with the more highly charged injected ions being slowed more efficiently than the less highly charged ions of the same species. However, if the process (1) has a large cross section, this separation will be greatly reduced. Similar considerations apply when one is concerned with the drift of ions through a plasma under the influence of an external field.

Asymptotic theories of ion-atom interactions[1-3] have been often used in calculations of cross sections for symmetric charge transfer in collisions of singly and doubly charged ions with their parent neutral atoms. The purpose of this paper is to show that these techniques can easily be adapted to give estimates of cross sections for symmetric charge transfer in ion-ion collisions.

For simplicity, let us assume that the reaction (1) involves a single valence electron and two closed-shell cores and that the transfer is between two ^2S states. The adaptation to other situations is straightforward.[1-6] The reaction is considered in terms of the formation and dissociation of a molecular ion, which can be in a gerade or ungerade state, with potentials $E_g(R)$ and $E_u(R)$. Atomic units will be used unless otherwise specified.

Using the impact-parameter approach, we consider the nuclei to move along classical trajectories determined by the average molecular potential-energy curve, and write the cross section as

$$\sigma(v)=2\pi\int_0^\infty P(b,v)b\,db \ . \tag{2}$$

$P(b,v)$ denotes the probability that charge transfer will occur during a collision with impact parameter b and relative velocity v. It can be expressed in terms of the difference between the gerade and ungerade potential curves

$$P(b,v)=\sin^2\left[\tfrac{1}{2}\int_{-\infty}^{\infty}\Delta E(R)dt\right]$$
$$=\sin^2\left[\int_\rho^\infty\frac{\Delta E(R)}{|dR/dt|}dR\right] , \tag{3}$$

where ρ is the distance of closest approach. Assuming that the average potential is dominated by the Coulomb interaction, this is given by the Rutherford scattering law[7]

$$\rho=b\left[\frac{\epsilon+1}{\epsilon-1}\right]^{1/2} , \tag{4}$$

with

$$\epsilon=\left[1+\left[\frac{2Eb}{p(p-1)}\right]^2\right]^{1/2} , \tag{5}$$

in which E is the relative energy of the colliding ions, and ϵ is the eccentricity of the orbit.

The integral in Eq. (3) is dominated by the region around $R=\rho$, since $\Delta E(R)$ decreases rapidly with increasing R and the denominator in the integrand vanishes at the classical turning point. For large impact parameters, such that $\epsilon\gg 1$, and R close to ρ, the radial velocity dR/dt can be approximated by

$$\left[\frac{dR}{dt}\right]^2=v^2\left[1-\frac{\rho^2}{R^2}\right] , \tag{6}$$

so that

$$P(b,v)=\sin^2\left[\frac{1}{v}\int_\rho^\infty\frac{\Delta E(R)}{(R^2-\rho^2)^{1/2}}R\,dR\right] . \tag{7}$$

This is equivalent to the formula used by Smirnov and co-workers[2,3] and by Hodgkinson and Briggs,[5] except that the impact parameter in their expression has been replaced by the distance of closest approach to allow for the curvature of the trajectory.

According to the asymptotic interaction theory, the molecular-energy difference $\Delta E(R)$ is approximately given by

$$\Delta E(R)=\frac{1}{R}\left[\frac{4}{e}\right]^n \psi^2\left[\frac{R}{2}\right], \tag{8}$$

where n is the effective quantum number, e is the base of natural logarithm, and $\psi(r)$ is the undistorted atomic radial wave function for the valence electron that is transferred. This is often fitted to the simple form

$$\psi(r)=qr^n\exp\left[-\frac{pr}{n}\right]. \tag{9}$$

The integral in Eq. (7) can be performed by the method of steepest descent through the substitution $R=\rho\cosh(x)$. This leads to

$$P(b,v)=\sin^2\left[\frac{q^2}{2v}\left[\frac{2\pi n}{p\rho}\right]^{1/2}\left[\frac{4\rho^2}{e}\right]^n\exp\left[-\frac{p\rho}{n}\right]\right]. \tag{10}$$

The integral over the impact parameter b can also be approximated using the Firsov procedure,[8]

$$\sigma(v)=\tfrac{1}{2}\pi b_0^2, \tag{11}$$

where b_0 is the largest value of the impact parameter for which

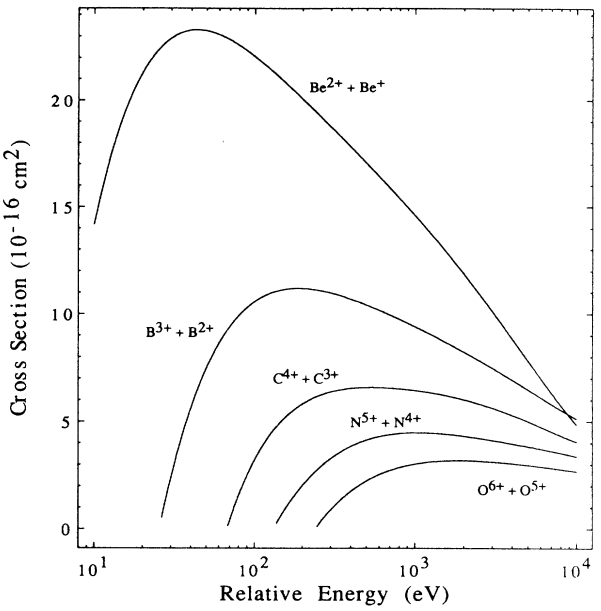

FIG. 2. Symmetric charge transfer cross sections for the Li-like ions.

$$P(b_0,v)=P_0. \tag{12}$$

The Firsov procedure reflects the rapid variation of the expression in square brackets in Eq. (10). For small impact parameters this expression is large and $P(b,v)$ oscillates rapidly with b, with an average value of 0.5. For large values of b the exponential factor decreases rapidly

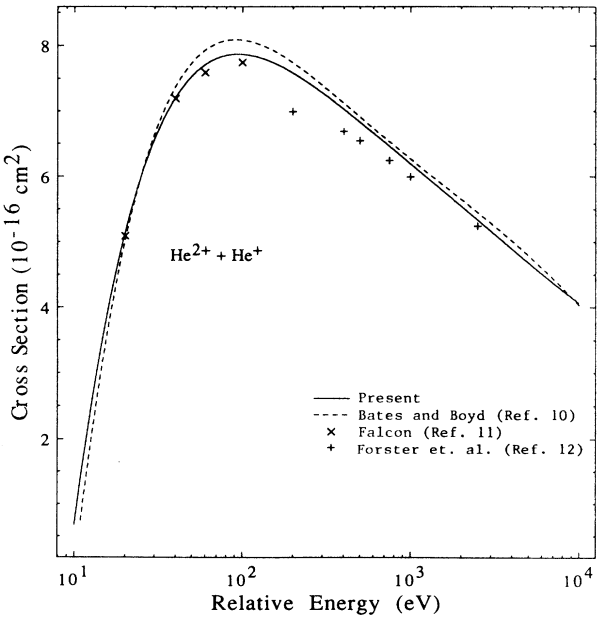

FIG. 1. Symmetric charge-transfer cross section for $He^{2+}+He^+\rightarrow He^++He^{2+}$.

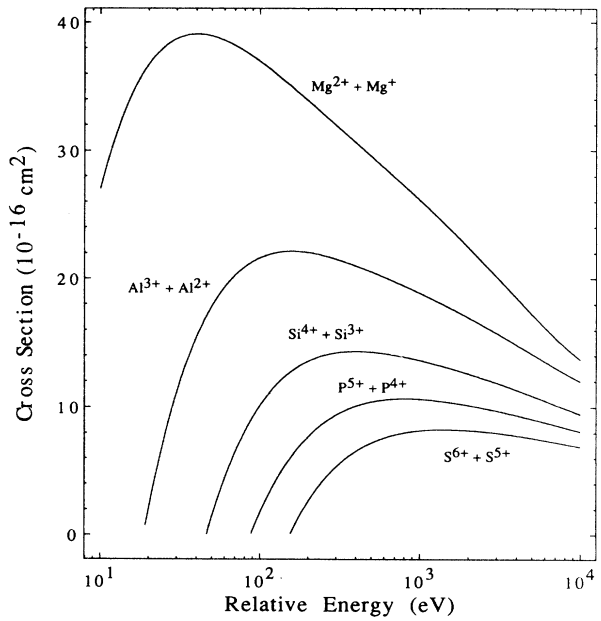

FIG. 3. Symmetric charge transfer cross sections for the Na-like ions.

and $P(b,v)$ is negligible. The steep decrease in $P(b,v)$ means that the calculated cross section is not very sensitive to the value chosen for P_0. We used the value of 0.075 recommended by Smirnov.[2,3]

The application of the asymptotic theory is very simple. First the constants n and q in Eq. (9) are obtained from the ionization potential and wave function for the valence electron. The value of the distance of closest approach ρ_0 corresponding to the critical impact parameter b_0 is then obtained from

$$\frac{q^2}{2v}\left[\frac{2\pi n}{p}\right]^{1/2}\rho_0^{2n-1/2}\exp\left[-\frac{p\rho_0}{n}-n\right]=0.28\ . \tag{13}$$

The cross section can then be found by computing b_0 from Eqs. (4) and (5) and using this value in Eq. (11).

For one-electron systems, such as He^+-He^{2+}, the potential curves $E_g(R)$ and $E_u(R)$ can be computed exactly.[9] Bates and Boyd[10] used exponential fits to the resulting energy differences in an impact-parameter calculation, using the Firsov approximation with $P_0=\sin^2(1/\pi)$. Our technique should be regarded as an extension to heavier systems of their pioneering work, in which exact potentials have been replaced by curves computed using asymptotic methods.

More accurate calculations for He^+-He^{2+} collisions have been reported by Falcon,[11] who performed quantum calculations between 20 and 100 eV, using the exact potential curves. The results, shown in Fig. 1, demonstrate that the two simple impact-parameter methods give excellent results in the region of overlap. Even at 10 eV, approximately 200 partial waves contribute to the cross section and the classical treatment of nuclear motion is justifiable. Although our results are in better agreement with the quantum values in the neighborhood of the maximum in the cross section, this is fortuitous since Bates and Boyd used more accurate potential curves. The differences at other energies are also not significant. At higher energies both impact-parameter calculations should become less accurate due to the failure of the Firsov approximation and the increasing strength of nonadiabatic effects.

Figure 1 also includes cross sections obtained by Forster *et al.*[12] using a semiclassical impact-parameter method with atomic orbitals modified by translation factors. Further study of the higher-energy regime would be worthwhile.

In Figs. 2 and 3 we present the cross sections obtained for the Li-sequence ions from Be^+ to O^{5+}, and for the Na-like ions from Mg^+ to S^{5+}. The only measurements of this process of which we are aware are for He^{2+}-He^+ by Jognaux *et al.*[13] and by Peart and Dolder.[14] It was concluded by Falcon[11] and by Dickinson and Hardie[15] that the acceptance angles of the detectors in those experiments were too small to give good estimates of the total cross sections. More experimental work on charge transfer in ion-ion collisions is strongly suggested.

This research was performed partly at Lawrence Livermore National Laboratory under the auspices of the U.S. Department of Energy through Contract No. W-7405-ENG-48.

[1]M. I. Chibisov and R. K. Janev, Phys. Rep. **166**, 1 (1988).
[2]E. E. Nikitin and B. M. Smirnov, Usp. Fiz. Nauk. **124**, 201 (1978) [Sov. Phys.—Usp. **21**, 95 (1978)].
[3]E. L. Duman and B. M. Smirnov, Teplofiz. Vys. Temp. **12**, 502 (1974) [High Temp. **12**, 431 (1975)].
[4]J. N. Bardsley, T. Holstein, B. R. Junker, and S. Sinha, Phys. Rev. A **11**, 1911 (1975).
[5]D. P. Hodgkinson and J. S. Briggs, J. Phys. B **9**, 255 (1976).
[6]S. Sinha and J. N. Bardsley, Phys. Rev. A **14**, 104 (1976).
[7]H. Goldstein, *Classical Mechanics* (Addison-Wesley, Reading, MA, 1980), pp. 108 and 109.
[8]O. B. Firsov, Zh. Eksp. Teor. Fiz. **21**, 1001 (1951).
[9]D. R. Bates, K. Ledsham, and A. L. Stewart, Philos. Trans. R. Soc. A **246**, 215 (1953).
[10]D. R. Bates and A. H. Boyd, Proc. Phys. Soc. **80**, 1301 (1962).
[11]C. A. Falcon, J. Phys. B **16**, 1793 (1983).
[12]C. Forster, R. Shingal, D. R. Flower, B.H. Bransden, and A. S. Dickinson, J. Phys. B **21**, 3941 (1988).
[13]A. Jognaux, F. Brouillard, and S. Szucs, J. Phys. B **11**, L669 (1978).
[14]B. Peart and K. Dolder, J. Phys. B **12**, 4155 (1979).
[15]A. S. Dickinson and D. W. Hardie, J. Phys. B **12**, 4147 (1979).